Variable-Fidelity Models in Optimization of Simulation-Based Systems

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Outline

- Introduction
- First-order model-management
  - Basic ideas
  - Example of an AMMO framework
  - Computational examples of design with variable-resolution, variable-fidelity physics models
    - 2D and 3D aerodynamic optimization with variable-resolution models
    - Multi-element airfoil design with variable-fidelity physics
    - 3D wing design with variable-fidelity physics
- Concluding remarks

Some Major Obstacles to Simulation-Based Design

- **Modeling**
  - **Simulation-based functions are expensive and not computationally robust**
  - **Difficult to obtain reliable and affordable derivatives**
- **Optimization**
  - **Algorithms for simulation-based design are in their infancy**

ASCoT Project (1998-2002)
(Aerospace Systems Concept to Test)

Project Vision

Physics-based modeling and simulation with sufficient speed and accuracy for validation and certification of advanced aerospace vehicle design in less than 1 year

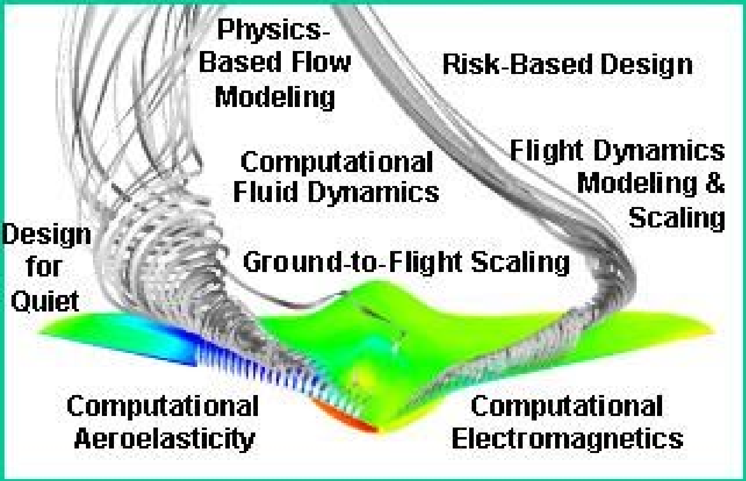
Project Goal

- **Provide next-generation analysis & design tools to increase confidence and reduce development time in aerospace vehicle designs**

Objective

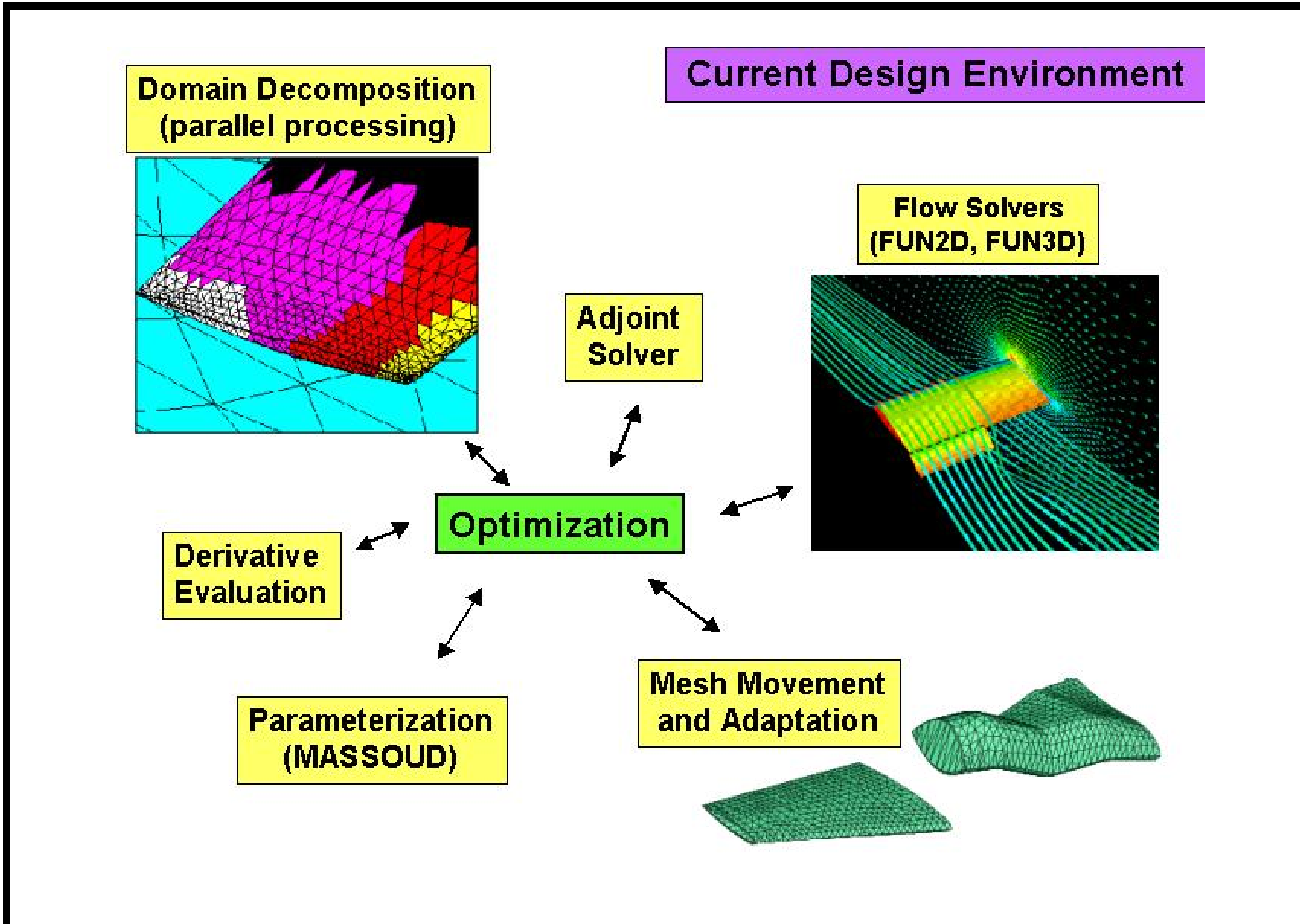
- Develop **fast, accurate, and reliable** analysis and design tools via fundamental technological advances in:
  - Physics-Based Flow Modeling
  - **Fast, Adaptive, Aerospace Tools (FAAST)** (CFD and Design)
  - Ground-to-Flight Scaling
  - Time-Dependent Methods
  - Design for Quiet
  - Risk-Based Design

Technology Areas



Benefit

- Increased Design Confidence
- Reduced Development Time

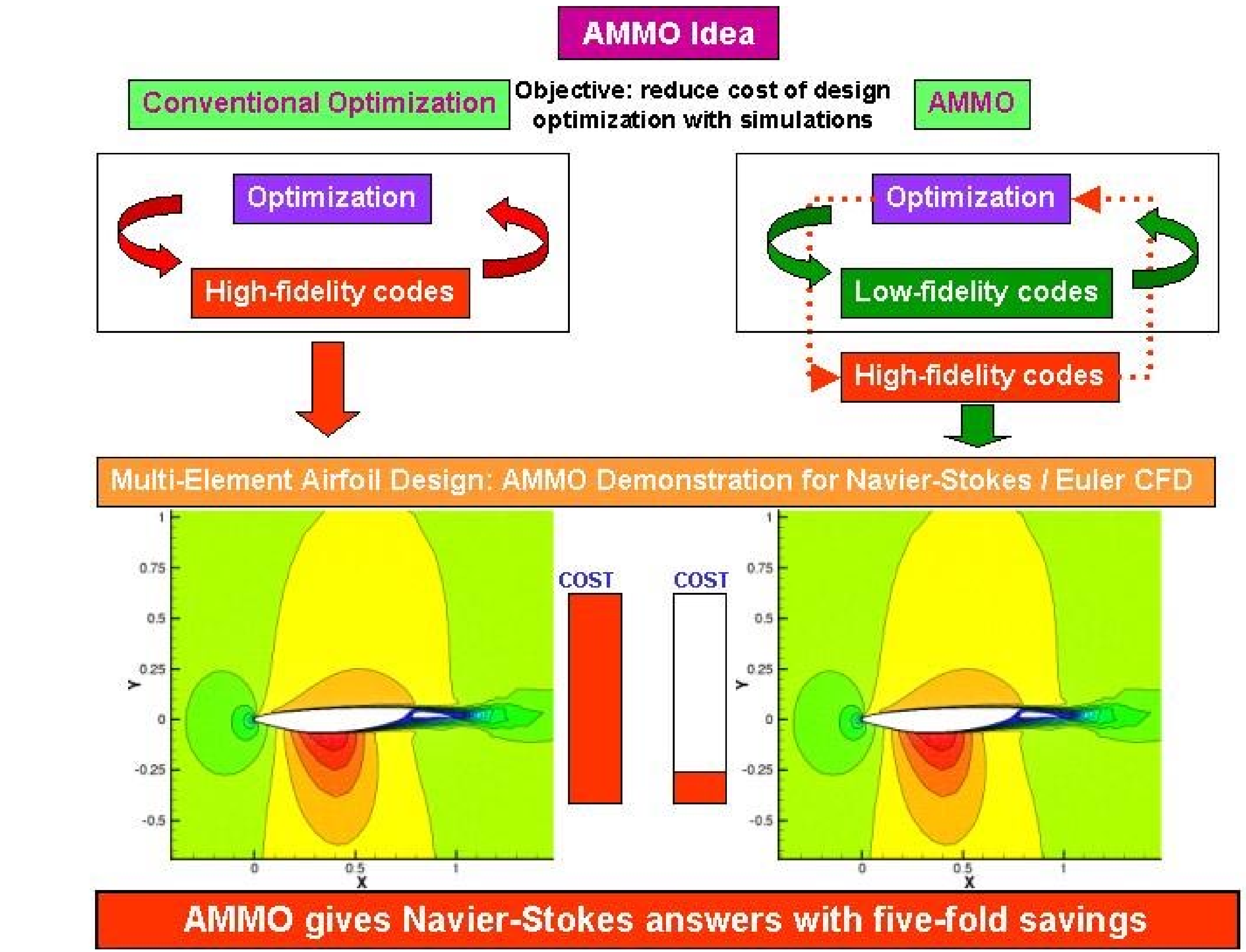

Current Design Environment
Domain Decomposition (parallel processing)
Flow Solvers (FUN2D, FUN3D)
Adjoint Solver
Optimization
Derivative Evaluation
Parameterization (MASSOUD)
Mesh Movement and Adaptation

Limiting Factors

- **Extreme expense of repeated simulations**
  - **Example: turbulent computation on 1 M grid points (Nielsen and Anderson)**
    - **1 day for submission, 3-4 days in queue**
    - **8 hours per 1 design cycle on 112 CPU**
    - **10 design cycles $\approx$ 9000 CPU hours for a simple single-point design**
- **Cost of solution is driven by simulations**
- **Function and derivative evaluations prone to failure away from nominal design**
- **Derivative-free optimization is not an option due to computational expense**

Approach

- **Engineering**
  - A variety of approximations and models available and used for a long time
  - *Ad hoc* optimization techniques
- **Mathematic Programming**
  - Generally limited to local Taylor series models
  - Rigorous and robust optimization techniques
- **Approximation and Model Management (AMMO)**
  - Use of Engineering approximations and models
  - Rigorous and robust optimization techniques
  - Can be used with any gradient-based algorithm


AMMO Idea
Conventional Optimization
Objective: reduce cost of design optimization with simulations
AMMO
Optimization
High-fidelity codes
Optimization
Low-fidelity codes
High-fidelity codes
Multi-Element Airfoil Design: AMMO Demonstration for Navier-Stokes / Euler CFD
COST
COST
AMMO gives Navier-Stokes answers with five-fold savings

Problem

- **The analysis or simulation problem:** Given x, solve a system of coupled equations

$$A(x, u(x)) = 0$$

for u that describes the physical behavior of the system.

- **The design problem (canonical formulation):** Solve

$$\begin{array}{ll} \underset{x}{\textbf{minimize}} & f(x, u(x)) \\ \textbf{subject to} & c_i(x, u(x)) = 0, \;\; i \in \mathcal{E} \\ & c_i(x, u(x)) \leq 0, \;\; i \in \mathcal{I} \\ & x_l \leq x \leq x_u, \end{array}$$

where, given x, $u(x)$ is determined from $A(x, u(x)) = 0$.

- In our context, "large-scale" means computationally expensive, regardless of the number of variables and constraints explicitly manipulated in optimization.

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Ensuring local similarity of trends

- **Convergence relies on ensuring local similarity of trends**

Let $\tilde{f}$, $\tilde{c}_E$, and $\tilde{c}_I$ be some lower-fidelity models of f, c_E and c_I, respectively. At each major iteration k, x_k of an AMMO algorithm, the models are required to satisfy first-order consistency:

$$\tilde{f}(x_k) = f(x_k), \qquad \tilde{c}_E(x_k) = c_E(x_k), \qquad \tilde{c}_I(x_k) = c_I(x_k)$$

$$\nabla \tilde{f}(x_k) = \nabla f(x_k), \qquad \nabla \tilde{c}_E(x_k) = \nabla c_E(x_k), \qquad \nabla \tilde{c}_I(x_k) = \nabla c_I(x_k)$$

- **Models with this property locally mimic the behavior of first-order Taylor-series models around x_k**

- **Easily enforced when derivatives are available**

Enforcing First-Order Consistency

- **Multiplicative "β-correction", Haftka, 1991:**
  - **Given $\phi_{hi}(x)$ (say, f) and $\phi_{lo}(x)$, define $\beta(x) \equiv \frac{\phi_{hi}(x)}{\phi_{lo}(x)}$**
  - **Given x_k, build $\beta_k(x) = \beta(x_c) + \nabla\beta(x_k)^T(x - x_k)$**
  - **Then $\tilde{\phi}_k(x) = \beta_k(x)\phi_{lo}(x)$ satisfies the consistency conditions at x_k**
- **Additive correction exist. For instance (Lewis and Nash, 2000):**

$$\tilde{\phi}_k(x) = \phi_{lo}(x) + [\phi_{hi}(x_k) - \phi_{lo}(x_k)] + [\nabla\phi_{hi}(x_k) - \nabla\phi_{lo}(x_k)]^T(x - x_k)$$

Examples of Variable-Fidelity Models for Use in AMMO

- **Data-fitting models (polynomial RS, splines, kriging)**
  - **Rely directly on hi-fi information; do not require derivatives; simple to construct; difficult to sample; "curse of dimensionality"**
- **Reduced-order models**
  - **Use reduced-order bases (constructed as a span of solutions and possibly derivatives at some points) to represent field variables at other points**
- **Variable-accuracy models**
  - **Converge analyses to a user-specified tolerance**
- **Variable-resolution models**
  - **Executing a single physical model on meshes of varying degree of refinement**
- **Variable-fidelity physics models**
  - **E.g., in aerodynamics, physical models range from inviscid, irrotational, incompressible flow to Navier-Stokes equations for nonlinear viscous flow**

Convergence vs. Performance

- **Convergence analysis relies on the consistency conditions and standard assumptions for the convergence analysis of the underlying algorithm (see paper for three examples)**
- **For convergence, need only a notion of two models, one arbitrarily designated "high fidelity" or "truth", the other - "low fidelity"**
- **Practical efficiency**
  - **Problem/model dependent**
  - **Depends on the ability to transfer computational load onto low-fidelity computation, which...**
  - **Depends on the predictive quality of the low-fidelity models (surrogates)**
  - **In the worst case, AMMO is conventional optimization**

Example: AMMO Based on Sℓ_1QP

- **AMMO can be used with any derivative-based algorithm; to date, implemented and tested AMMO based on five algorithms**
- **Principle: a simple implementation with maximum use or existing software**
- **Problem: have not found software suitable for simulation-driven optimization**
- **Resolution: writing our own**
- **Meanwhile: nonsmooth exact penalty functions - a potential alternative to SQP; simple merit function, similar convergence properties (Fletcher 1989)**

Consider a composite penalty function

$$\mathcal{P}(x;h) \equiv f(x) + h(c(x)),$$

where f and c are smooth and h is convex but possibly only continuous.

Sℓ_1QP

Fletcher's choice of $\mathcal{P}$ is the penalty function

$$\mathcal{P}(x;\sigma) = f(x) + \sigma \sum_{i\in E} |c_i(x)| + \sigma \sum_{i\in I} \max\{0, c_i(x)\}.$$

This is an exact penalty function if σ satisfies

$$\sigma > \min_{i\in L} |\lambda_i|,$$

where L is the set of all multipliers for the NLP. The model of $\mathcal{P}$ is

$$m(x_k, s; \sigma) \equiv q(x_k, s) + \sigma \sum_{i\in E} |l_i(x_k, s)| + \sigma \sum_{i\in I} \max\{0, l_i(x_k, s)\},$$

where $q(x_k, s)$ is the quadratic model of f and $l_i(x_k, s)$ are linearizations of constraints. The prototype Sℓ_1QP finds global solutions s_k of

$$\begin{aligned} &\underset{s}{\textbf{minimize}} && m(x_k, s; \sigma) \\ &\textbf{subject to} && \| s \|_\infty \le \Delta_k \end{aligned}$$

Sℓ_1QP, continued

The step is evaluated by examining

$$\rho_k = \frac{\mathcal{P}(x_k;\sigma_k) - \mathcal{P}(x_k + s_k;\sigma_k)}{m(x_k, 0;\sigma_k) - m(x_k, s_k;\sigma_k)}$$ **as follows:**

Select $0 < r_1 < r_2 \leq 1$ **and** $0 < \kappa_1 < 1 < \kappa_2$.
Typical values are $r_1 = 0.25$, $r_2 = 0.75$, $\kappa_1 = 0.25$, $\kappa_2 = 2$.

Set $x_{k+1} = \begin{cases} x_k & \text{if } \rho_k \leq 0 \\ x_k + s_k & \text{otherwise.} \end{cases}$

Set $\Delta_k = \begin{cases} \kappa_1 \| s_k \| & \text{if } \rho_k < r_1 \\ \kappa_2 \Delta_k & \text{if } \rho_k > r_2 \text{ and } \| s_k \| = \Delta_k \\ \Delta_k & \text{otherwise.} \end{cases}$

Sℓ_1QP-AMMO Model and Algorithm

$$m(k, x_k, s; \sigma) \equiv \tilde{f}(k, x_k, s) + \sigma \sum_{i \in E} |\tilde{c}_{E,i}(k, x_k, s)| + \sigma \sum_{i \in I} \max\{0, \tilde{c}_{I,i}(k, x_k, s)\}$$

whose components satisfy the consistency conditions. Note that the model m depends on k. as follows.

Initialization: Choose x_0, Δ_0, and constants as above.

Do $k = 0, 1, \ldots$ until convergence:

Model construction:

Construct model $m(k, x_k, s; \sigma_k)$ of $\mathcal{P}$

Step computation:

Solve for s_k $\begin{cases} \text{minimize}_{s} & m(k, x_k, s; \sigma_k) \\ \text{subject to} & \| s \| \leq \Delta_k \end{cases}$

Step evaluation: Compute ρ_k. Accept or reject the step based on ρ_k as above.

Updates: Update x_k, Δ_k based on ρ_k as above.

End do

Convergence of Sℓ_1QP-AMMO

Theorem:

Let $f, c_E, c_I \in C^2(\Omega)$ have bounded second derivatives on a bounded $\Omega \subset I\!R^n$. Let $\tilde{f}, \tilde{c}_E, \tilde{c}_I \in C^2(\Omega)$ be any models of f c_E, and c_I, respectively, that satisfy the first order consistency conditions and have uniformly bounded second derivatives on Ω. Let $\{x_k\} \in \Omega$ be the sequence of iterates generated by Sℓ_1QP–AMMO. The there exists an accumulation point x_* at which the first-order optimality conditions for minimizing $\mathcal{P}$ hold, that is,

$$\underset{\lambda \in \partial h_*}{\textbf{maximize}} \ (g_* + \nabla c_* \lambda)^T s \geq 0 \text{ for all } s,$$

where ∂h_* is the generalized derivative of h.

An Alternative Sℓ_1QP-AMMO

Impose the following conditions on the model and the trial step:

- **Smoothness:** The model m is locally Lipschitz continuous and regular with respect to s for all (x, σ) and continuous in (x, σ) for all s.
- **Zero-order matching:** The values of the function and model coincide when $s = 0$.
- **First-order matching:** The generalized directional derivatives of the function and model coincide when $s = 0$.
- **Bounded parameters:** The set of problem parameters is closed and bounded.
- **Sufficient decrease:** For any x_*, there exist constants $\delta, \epsilon, \kappa \in (0, 1)$ such that s_k satisfies

$$m(k, x_k, 0, \sigma_k) - m(k, x_k, s_k, \sigma_k) \geq \kappa \parallel g(x_k) \parallel \min\{\delta, \Delta_k\},$$

where $g = \arg\min_{g \in \partial f} \parallel g \parallel$. These conditions are summarized in CGT 2000.

An Alternative Sℓ_1QP-AMMO, continued

In Sℓ_1QP-AMMO, the smoothness, boundedness, zero- and first-order matching conditions are satisfied by assumption. Guaranteeing sufficient decrease - in progress.

Updates for Sℓ_1QP-AMMO with sufficient decrease

Select $\Delta_{max} > 0, 0 < r_1 \leq r_2 \leq 1$ **and** $0 < 1/\kappa_3 \leq \kappa_1 \leq \kappa_2 < 1 < \kappa_3$.

$$\text{Set } (x_{k+1}) = \begin{cases} x_k + s_k & \text{if } \rho_k \geq r_1 \\ x_k & \text{otherwise.} \end{cases}$$

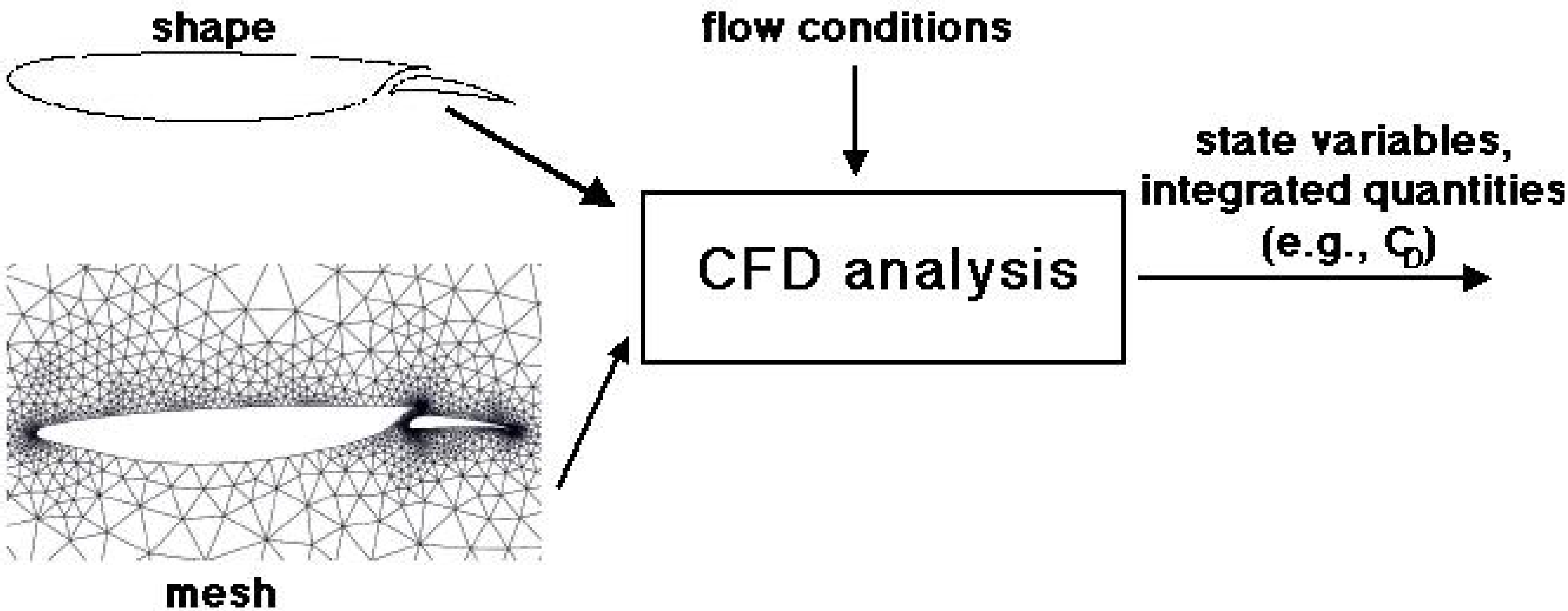
$$\text{Set } \Delta_{k+1} \in \begin{cases} [\kappa_1 \Delta_k, \kappa_2 \Delta_k] & \text{if } \rho_k < r_1 \\ [\kappa_2 \Delta_k, \Delta_k] & \text{if } \rho_k \in [r_1, r_2) \\ [\kappa_3 \Delta_k, \kappa_2 \Delta_{max}] & \text{if } \rho_k \geq r_2. \end{cases}$$

Convergence to a first-order critical point is immediate under these conditions (see, e.g., Theorem 11.2.5 in CGT 2000).

Computational Demonstrations

- **Because of data-fitting model limitations, we have focused on models that are independent of the number of variables**
- **Independence wrt dimension is important: in preliminary design, problems of modest size number O(100) variables**
- **AMMO admits a wide variety of models and algorithms; demonstrations are aimed at accumulating realistic experience to validate the algorithmic performance**
- **Because we cannot predict *a priori* the relative descent characteristics of models, must include cases of favorable and unfavorable relationship between models**
- **Aerodynamic shape optimization is a good test problem: practically important, computationally intensive, comes in a variety of dimensions**

Demonstration Problems: Aerodynamic Optimization



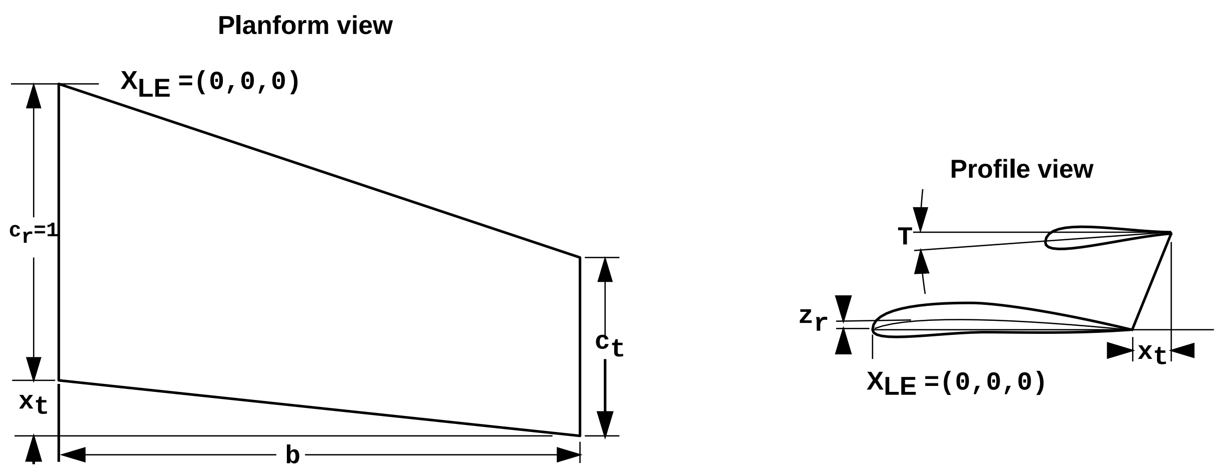
minimize Integrated quantities, such as $-\frac{L}{D}$ $\left(\frac{\text{lift}}{\text{drag}}\right)$or C_D (drag coefficient)

subject to constraints on, e.g., pitching and rolling moment coefficients, etc.

$x_l \leq x \leq x_u$

Managing Variable-Resolution Models:
(AIAA-2000-0841, Alexandrov, Lewis, Gumbert, Green, Newman)

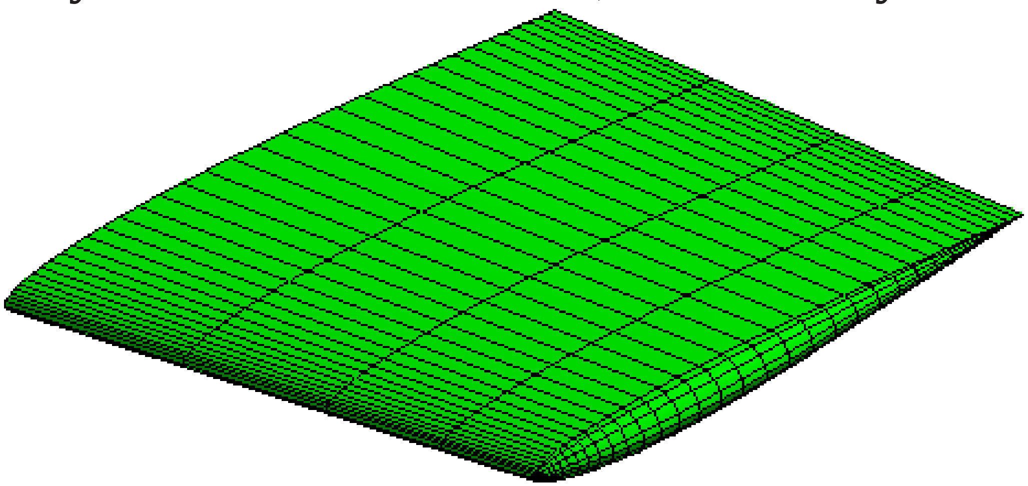
- **Analysis: Euler (NS/Euler code CFL3D, Rumsey et al., NASA LaRC)**
- **Conditions: $M_\infty = 0.6, \alpha = 3.0$**
- **Design variables: tip chord, tip trailing edge setback**



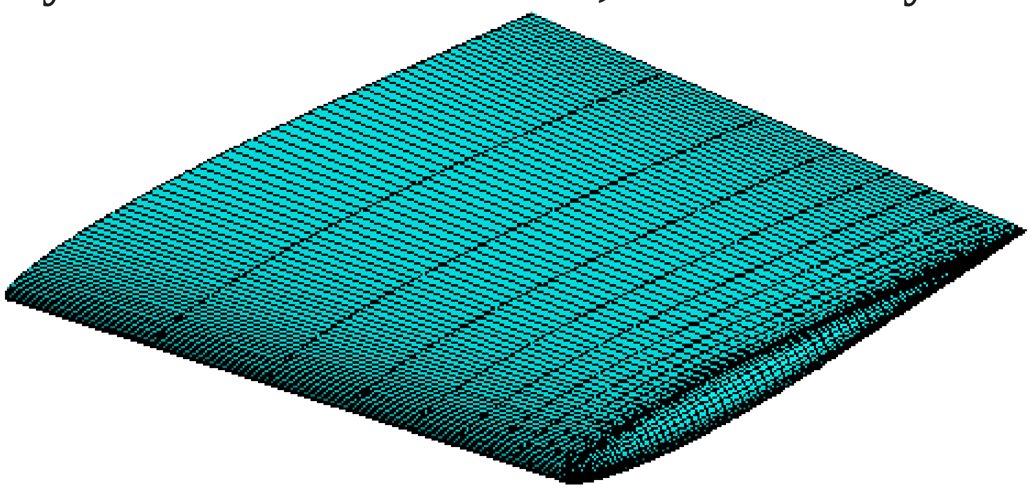
- **Objective: $-\frac{L}{D}$**
- **Constraints in lieu of multidisciplinary constraints: a lower bound on total lift $C_L S$, upper bounds on the pitching moment coefficient C_M and the rolling moment coefficient C_l**

3D Wing Optimization: Problem Description

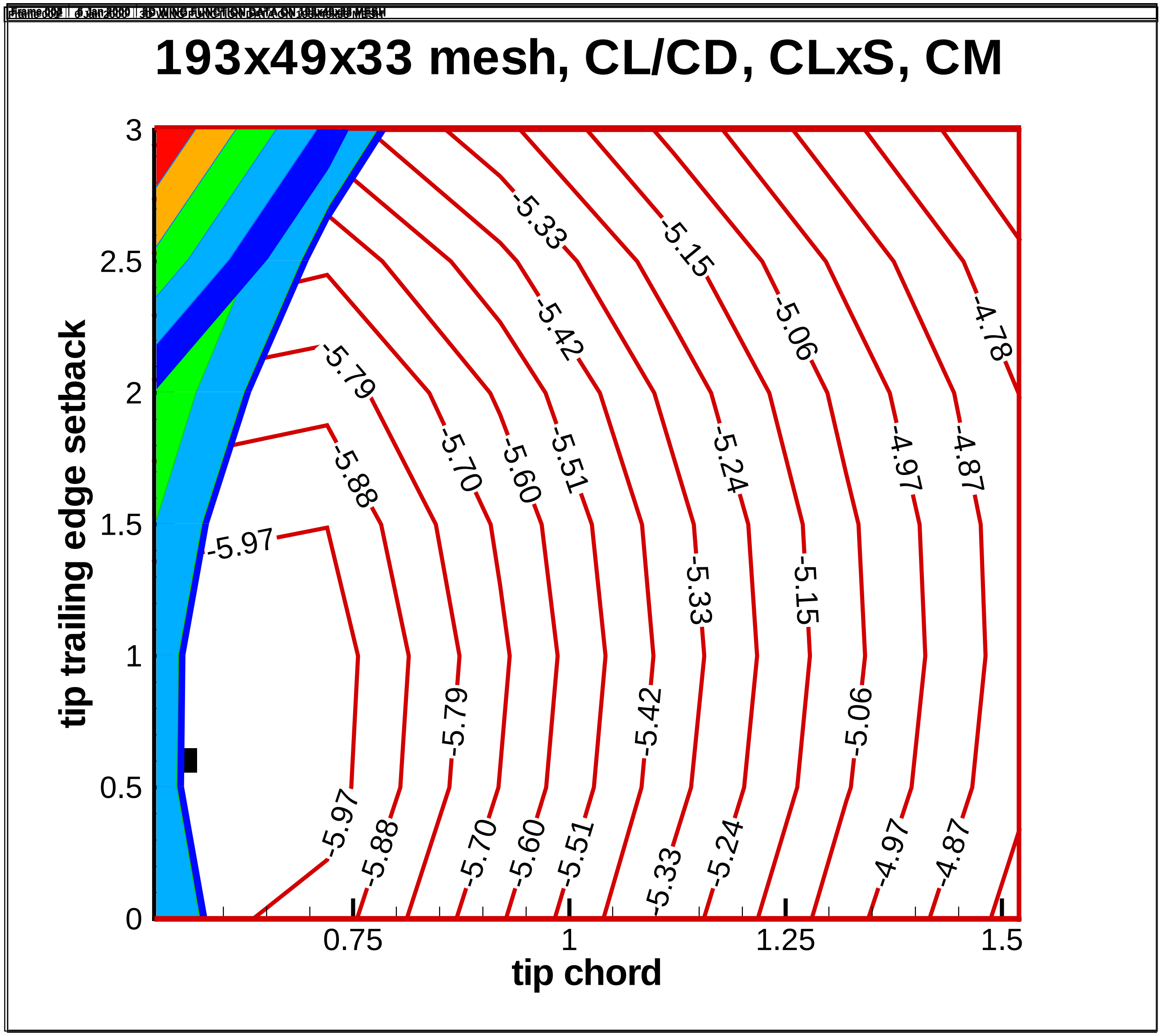
Low-fidelity: analysis on 97x25x17 mesh, 8 min/analysis on Sun SPARC 1:



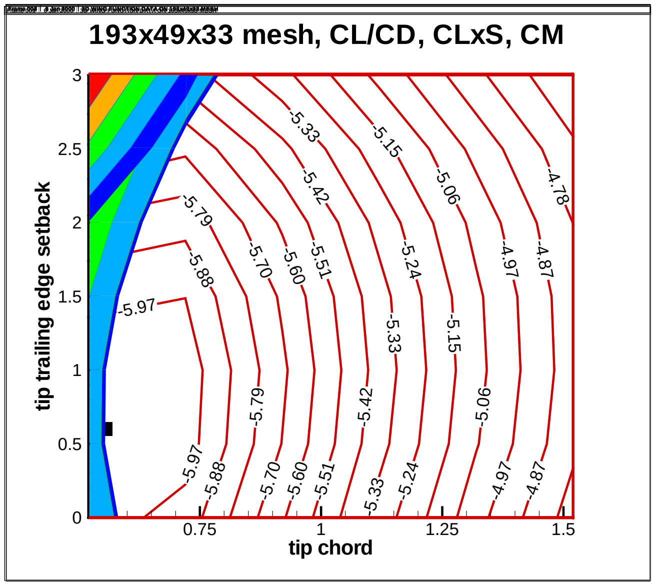
High-fidelity: analysis on 193x49x33 mesh, 64 min/analysis on Sun SPARC 1:

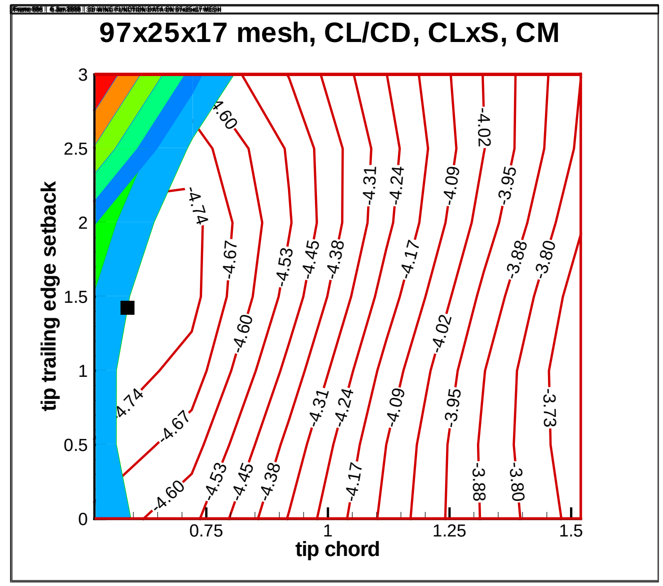


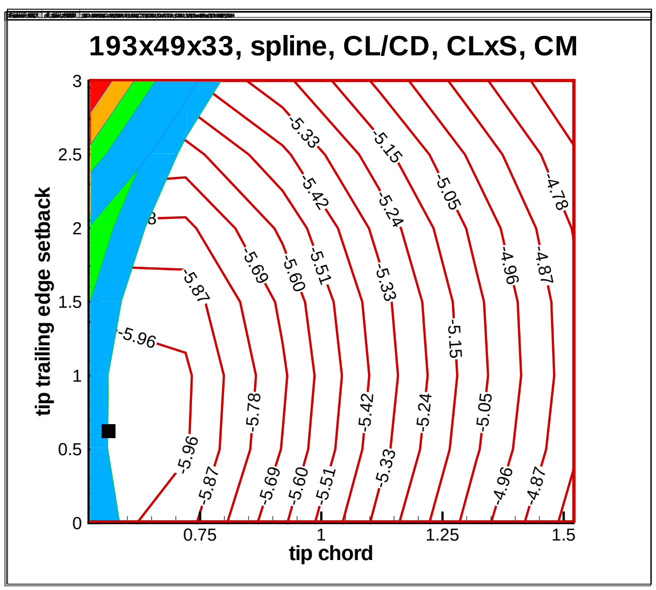
3D Wing Optimization: Problem Level Sets, Example

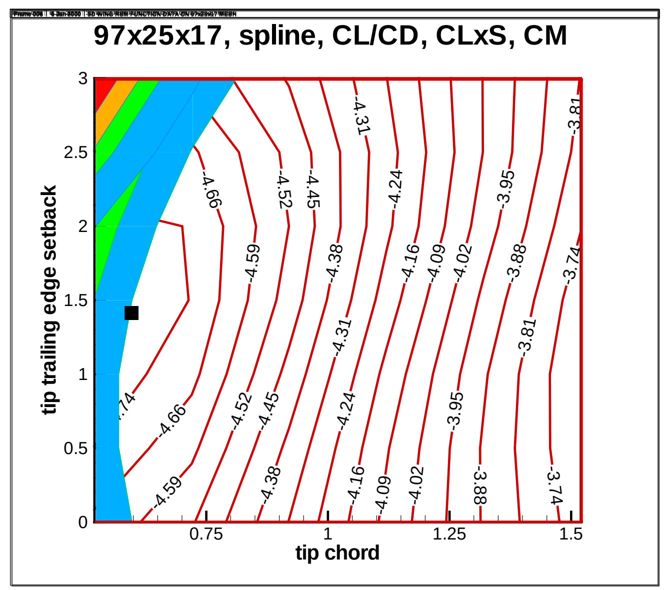


3D Wing Optimization: Actual Functions vs. Spline Substitutes

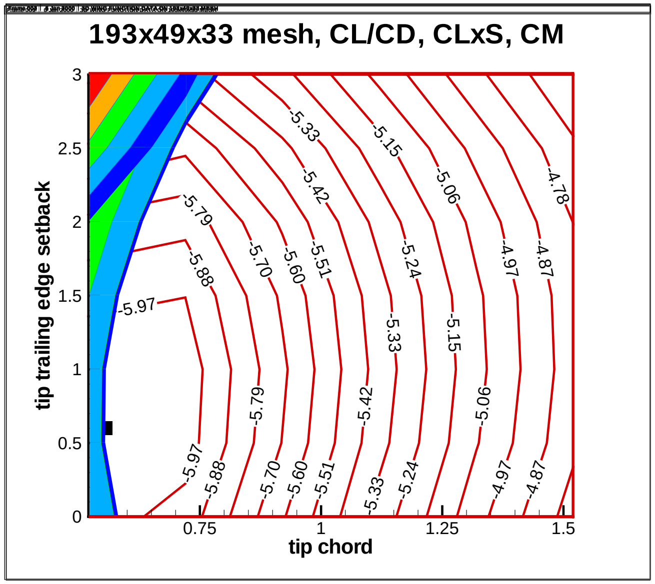


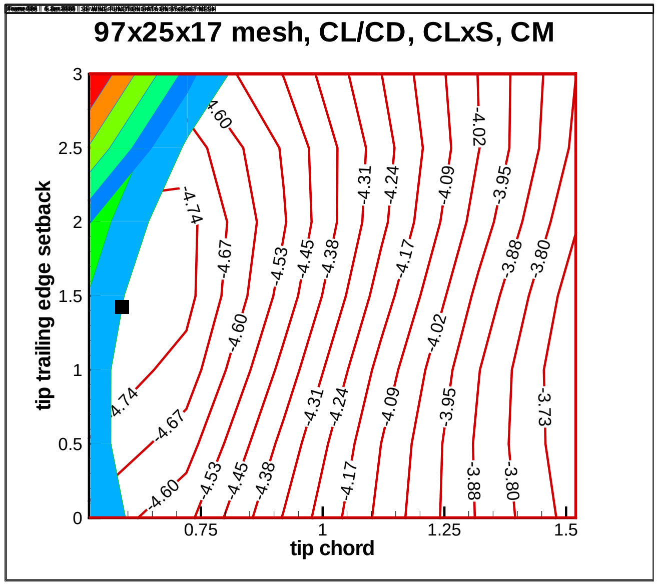


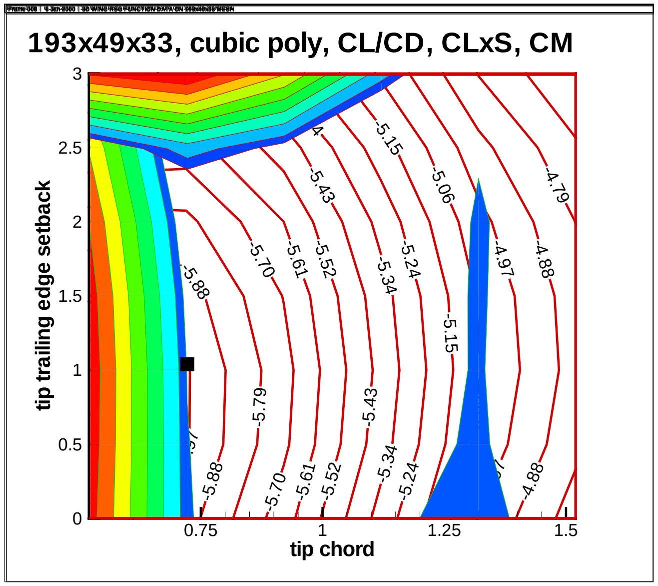


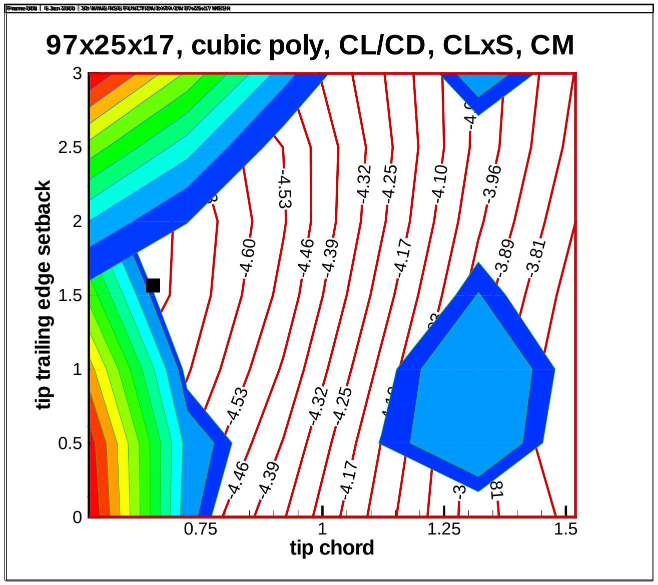


3D Wing Optimization: Actual Functions vs. Cubic Polynomial Substitutes









3D Wing Optimization: Discussion of Results

- Function evaluations, conventional SQP vs. SQP-AMF (number of sensitivity evaluations - same):

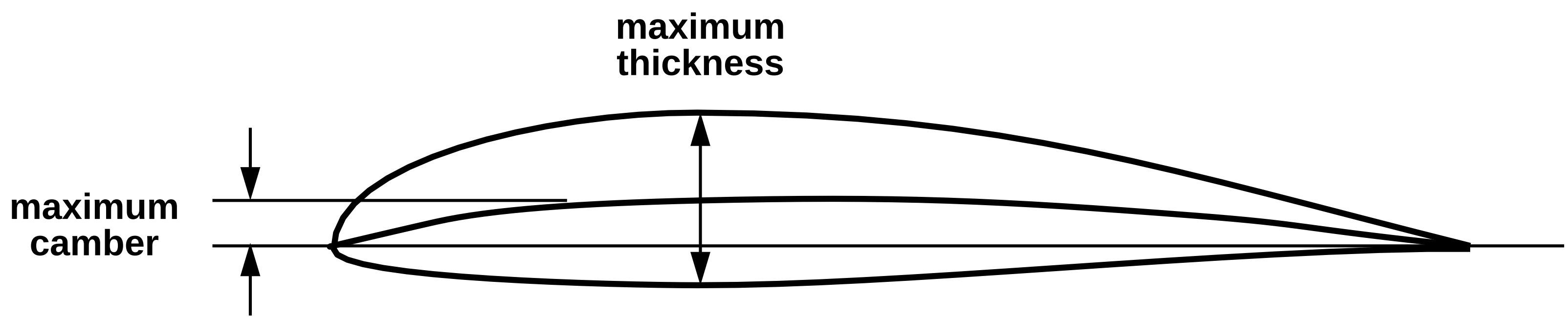
	hi-fi eval	lo-fi eval	equiv hi-fi eval	factor
Conventional SQP on poly	31		31	
SQP-AMF on poly	4	51	4 + 51/8 = 10 3/8	2.99
Conventional SQP on splines	21		21	
SQP-AMF on splines	4	28	4 + 28/8 = 7 1/2	2.8

- Optimization convergence criterion: 10^{-5}
- Optimization was done on RSM substitutes
- Savings across methods similar

2D Airfoil Optimization: Problem Description

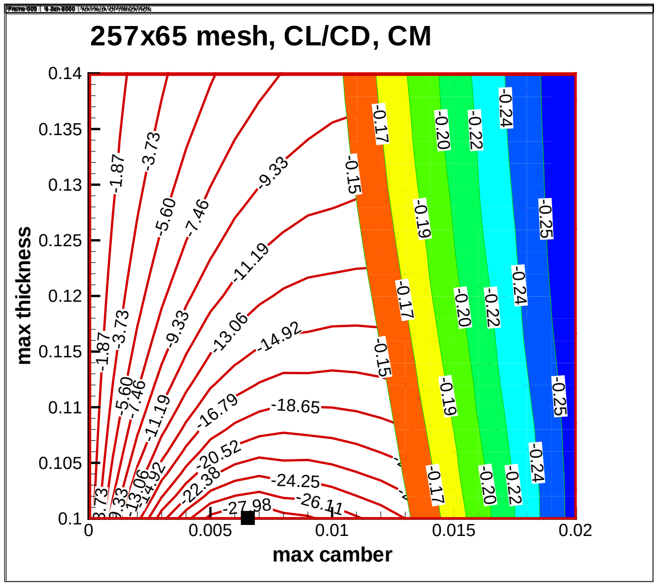
Problem formulated and assembled by L.L. Green

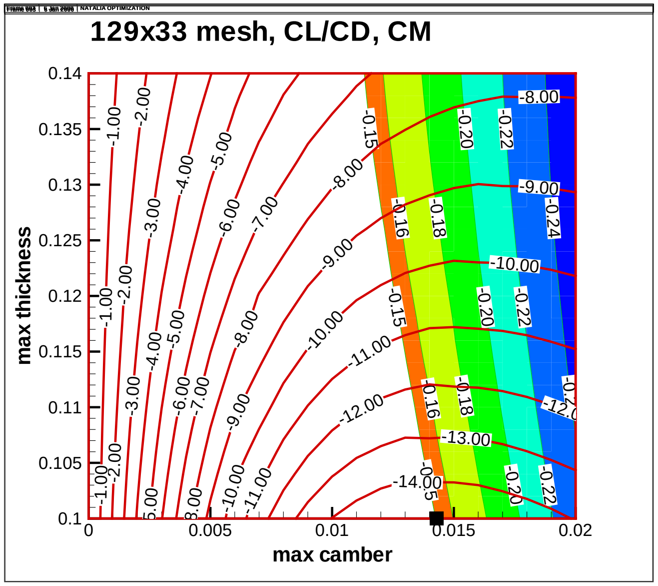
- Analysis: Euler (NS/Euler code FLOMG, Swanson, Turkel)
- Design variables:



- Objective: $-\frac{L}{D}$
- Constraints: pitching moment
- Levels of fidelity: analyses on 257x65 and 129x33 meshes
- Time/analysis on 257x65 mesh = 4 Time/analysis on 129x33 mesh
- Approximately 8 min vs 2 min per analysis on SGI Octane

2D Airfoil Optimization: Discussion of Results





- **Savings in function/sensitivity evaluations approximately twofold (factor ranging from 2.2 to 3.1) across all methods**
- **Savings lower than for the 3D wing problem due to lower computational expense**

Managing Variable-Fidelity Physics Models: Multi-Element Airfoil

(AIAA-2000-4886, Alexandrov, Nielsen, Lewis, Anderson)

- A two-element airfoil designed to operate in a transonic regime — inclusion of viscous effects is very important
- Governing equations: time-dependent Reynolds-averaged Navier-Stokes

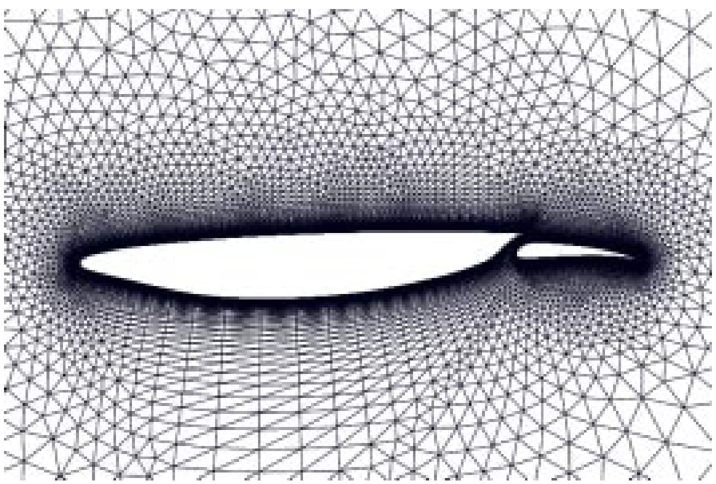
$$A\frac{\partial Q}{\partial t} + \oint_{\partial\Omega} \vec{F}_i \cdot \hat{n}dl - \oint_{\partial\Omega} \vec{F}_v \cdot \hat{n}dl = 0,$$

  where $\vec{F}_i$ and $\vec{F}_v$ are the inviscid and viscous fluxes, respectively
- Flow solver (FUN2D) – unstructured mesh methodology (Anderson, 1994)
- Sensitivity derivatives – hand-coded adjoint approach (Anderson, 1997)
- Conditions:
  - $M_\infty = 0.75$
  - $Re = 9 \times 10^6$
  - $\alpha = 1^\circ$ (global angle of attack)

Multi-Element Airfoil, cont.

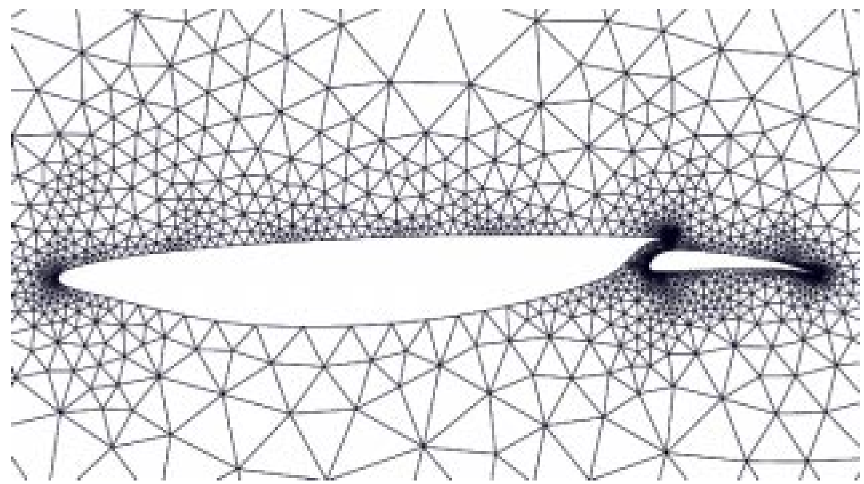
- **Hi-fi model – FUN2D analysis in RANS mode**
- **Lo-fi model – FUN2D analysis in Euler mode**
- **Computing on SGI Origin^{TM} 2000, 4 R1OK processors**

Viscous mesh:
10449 nodes and 20900 triangles



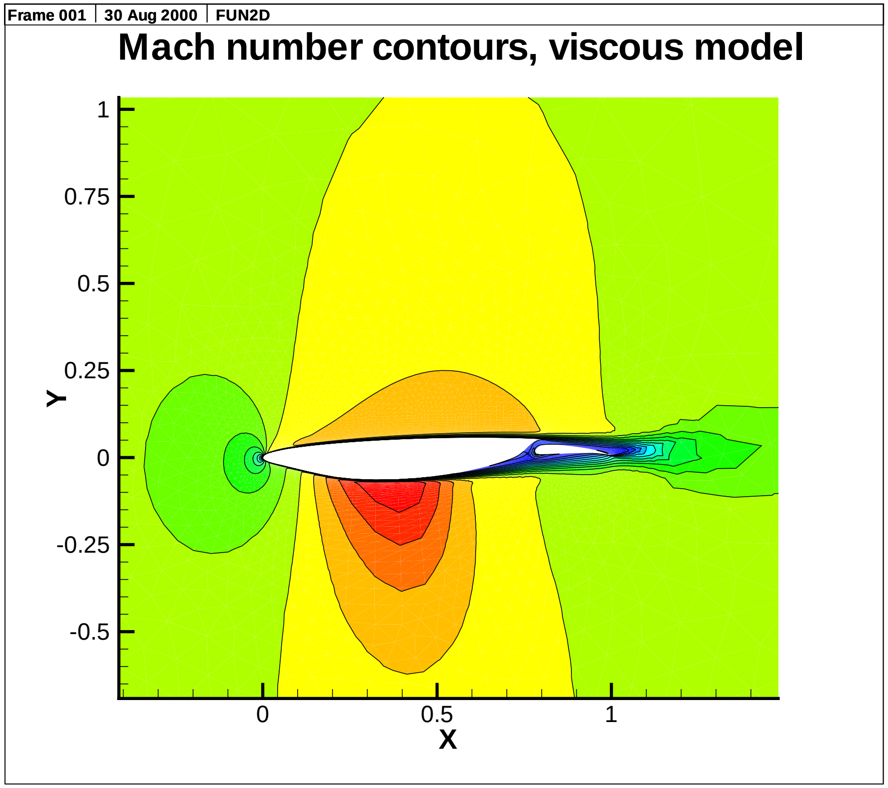
t/analysis $\approx$ 21 min
t/sensitivity $\approx$ 21 or 42 min

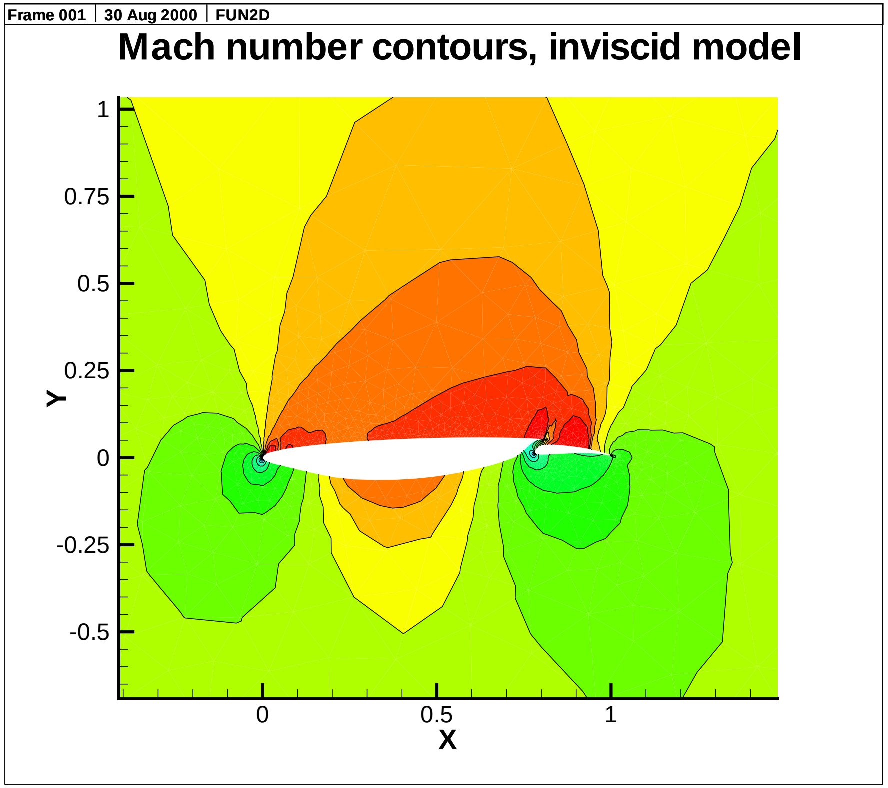
Inviscid mesh:
1947 nodes and 3896 triangles



t/analysis $\approx$ 23 sec
t/sensitivity $\approx$ 100 or 77 sec

Multi-Element Airfoil: Viscous Effects





- **Boundary and shear layers are visible in the viscous case.**

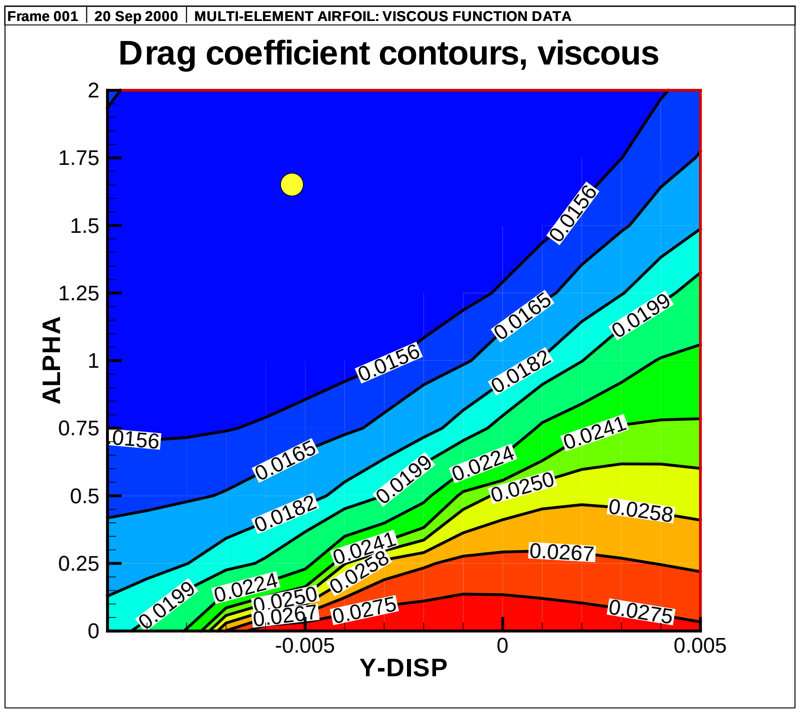
Multi-Element Airfoil: Computational Experiments

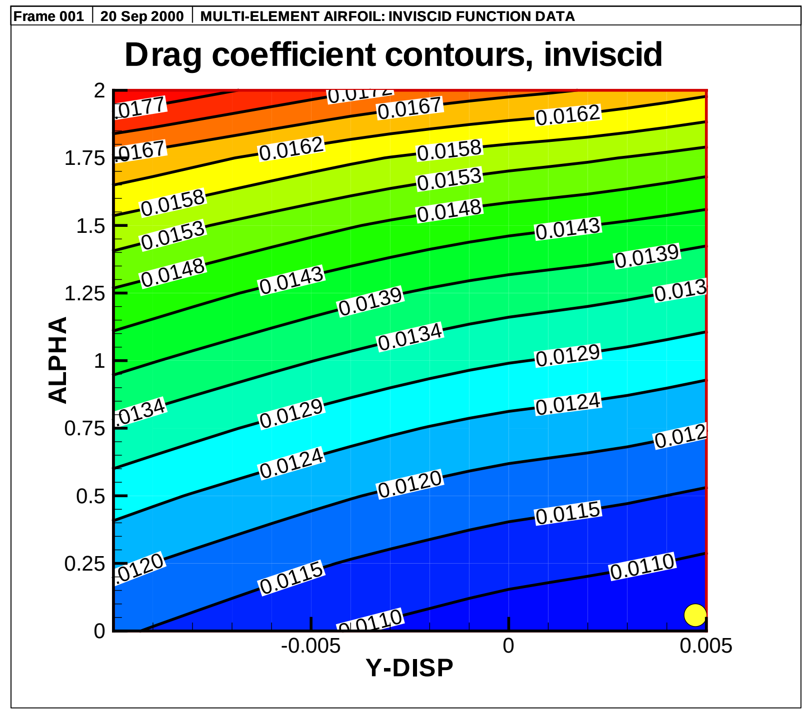
- **Objective function:** minimize drag coefficient subject to bounds on variables
- **Case 1:** (for visualization)
  - Variables: angle of attack, y-displacement of the flap
  - Solve problem with hi-fi models alone using a commercial optimization code (PORT, Bell Labs)
  - Solve the problem with AMMO, PORT used for lo-fi subproblems
- **Case 2:**
  - Variables: angle of attack, y-displacement of the flap, geometry description of the airfoil; 84 variables total
  - Same experiment

Multi-Element Airfoil: Models

- **Time/function for inviscid model negligible compared to viscous model**

- **Descent trends are reversed — unusual but a good test**

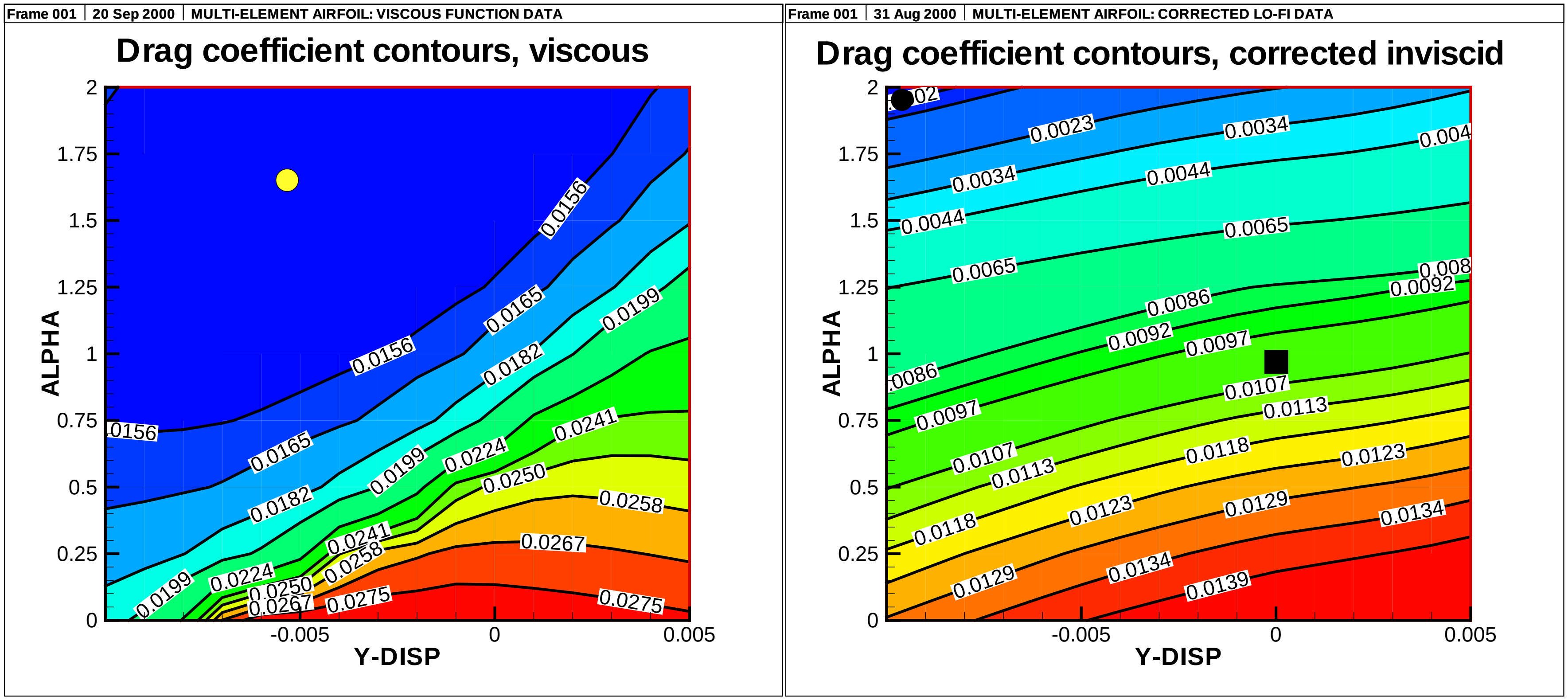




Multi-Element Airfoil: AMMO Iterations with 2 Variables

Iteration 1. **Starting point:** $\alpha = 1.0$, **y-disp** $= 0.0$

High-fidelity objective vs. corrected low-fidelity objective



New point: $\alpha = 2.0$, **y-disp** $= -0.01$

Multi-Element Airfoil: AMMO Iterations with 2 Variables, cont.

- **Similar effect in the next iteration**
- **Solution ($\alpha = 1.6305°$, flap y-displacement $= -0.0048$) located at iteration 2**
- $C_D^{\text{initial}} = 0.0171$ **at ($\alpha = 1°$, flap y-displacement $= 0$)**
- $C_D^{\text{final}} = 0.0148$**, a decrease of approximately** 13.45%**.**

Multi-Element Airfoil: Performance Summary

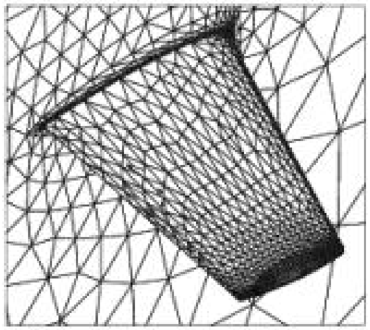
Notation: No. functions / No. Gradients

Test	hi-fi eval	lo-fi eval	total t	factor
PORT with hi-fi analyses, 2 var	14/13		$\approx$ 12 hrs	
AMMO, 2 var	3/3	19/9	$\approx$ 2.41hrs	$\approx$ 5
PORT with hi-fi analyses, 84 var	19/19		$\approx$ 35 hrs	
AMMO, 84 var	4/4	23/8	$\approx$ 7.2hrs	$\approx$ 5

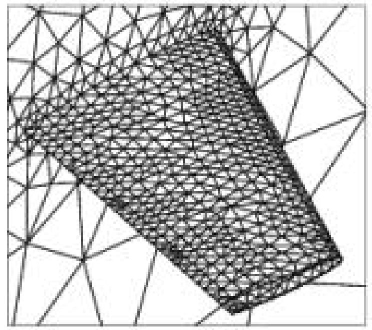
Current Results (with E. J. Nielsen)

3D Aerodynamic Design with AMMO

Hi-fi: FUN3D N-S on a finer mesh



Lo-fi: FUN3D Euler on a coarse mesh



$$\min_x \quad 5C_D^2 + \tfrac{1}{2}(C_L - 0.12303)^2$$
$$s.t. \quad x_l \le x \le x_u$$

α_0=3.06°, M_∞=0.84, Re=5x10^6

$\text{Lift}_0 = 0.12302$, $\text{Drag}_0 = 0.01713$, $\text{Objective}_0 = 0.0014670$

Cost Reduction with AMMO
(No. functions / No. gradients)

Test	Hi-fi eval	Lo-fi eval	Final Lift	Final Drag	f
PORT/hi-fi	13/11		0.11146	0.01532	0.0012793
AMMO	3/3	22/15	0.10657	0.01511	0.0012796

- Factor 2 savings in terms of wall-clock time
- Further savings are expected upon development of optimal termination criteria for low-fidelity subproblem computations
- Large-scale 3D slot wing design in progress

Work in Progress

- **Computational expense is still a difficulty**
  - **Investigating optimal termination of the low-fidelity computations based on sufficient predicted decrease**
  - **Investigating MASSOUD (J.A. Samareh) as a potential robust and efficient volume grid manipulation tool**
  - **Choice of “optimal” models**
- **Explicit constraint handling in optimization problems**
  - **Complex derivatives**
  - **Adjoints when design variables outnumber responses**
- **Handling mesh adaptation or regenerating meshes in optimization**
- **Robust handling of analysis and mesh movement failure**

Some Publications on First-Order Model Management:

Alexandrov, N. M.; Lewis, R. M.: "First-Order Model Management for Engineering Optimization", Optimization and Engineering, 2001, in press.

Alexandrov, N. M.; Lewis, R. M.: "First-Order Approximation and Model Management in Optimization", Large-Scale PDE-Constrainted Optimization, 2001, Springer-Verlag, Berlin, in press.

Alexandrov, N. M.; Nielsen, E. J.; Lewis, R. M.; Anderson, W. K.: "First-Order Model Management with Variable-Fidelity Physics Applied to Multi-Element Airfoil Optimization", AIAA Paper 2000-4886, 8th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Long Beach, CA, 6-8 Sept. 2000; also Journal of Aircraft, in press. LTRS.

Alexandrov, N. M.; Lewis, R. M.; Gumbert, C. R.; Green, L. L.; and Newman, P.A.: "Optimization with Variable-Fidelity Models Applied to Wing", AIAA Paper 2000-0841, 38th Aerospace Sciences Meeting and Exhibit, 10-13 January 2000, Reno, NV. LTRS.

Alexandrov, N.: "On Managing the Use of Surrogates in General Nonlinear Optimization and MDO", AIAA Paper 99-4798, 7th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, St. Louis, MO, Sept. 2-4, 1998. LTRS

Alexandrov, N.: "A Trust-Region Framework for Managing Approximations in Constrained Optimization and MDO Problems", ISSMO/NASA 1st Internet Conference on Approximations and Fast Re-Analysis in Engineering Optimization, June 14-27, 1998.